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TERMINAL (ENTER 1, 2, 3, OR ?):2

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* * * * * * * * * *
                     Welcome to STN International
                                                   * * * * * * * * * *
NEWS
                 Web Page for STN Seminar Schedule - N. America
NEWS 2 OCT 02 CA/CAplus enhanced with pre-1907 records from Chemisches
                 Zentralblatt
NEWS 3 OCT 19 BEILSTEIN updated with new compounds
NEWS 4 NOV 15 Derwent Indian patent publication number format enhanced
NEWS 5 NOV 19 WPIX enhanced with XML display format
NEWS 6 NOV 30 ICSD reloaded with enhancements
NEWS 7 DEC 04 LINPADOCDB now available on STN
NEWS 8 DEC 14 BEILSTEIN pricing structure to change
NEWS 9 DEC 17 USPATOLD added to additional database clusters
NEWS 10 DEC 17 IMSDRUGCONF removed from database clusters and STN
NEWS 11 DEC 17 DGENE now includes more than 10 million sequences
NEWS 12 DEC 17 TOXCENTER enhanced with 2008 MeSH vocabulary in
                 MEDLINE segment
NEWS 13 DEC 17 MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS 14 DEC 17 CA/CAplus enhanced with new custom IPC display formats
NEWS 15 DEC 17 STN Viewer enhanced with full-text patent content
                 from USPATOLD
NEWS 16 JAN 02
                 STN pricing information for 2008 now available
NEWS 17 JAN 16 CAS patent coverage enhanced to include exemplified
                 prophetic substances
NEWS 18 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new
                 custom IPC display formats
NEWS 19 JAN 28 MARPAT searching enhanced
NEWS 20 JAN 28 USGENE now provides USPTO sequence data within 3 days
                 of publication
NEWS 21 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 22 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements
NEWS 23 FEB 08 STN Express, Version 8.3, now available
NEWS 24 FEB 20 PCI now available as a replacement to DPCI
NEWS 25 FEB 25 IFIREF reloaded with enhancements
NEWS 26 FEB 25 IMSPRODUCT reloaded with enhancements
NEWS 27 FEB 29 WPINDEX/WPIDS/WPIX enhanced with ECLA and current
                 U.S. National Patent Classification
NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
```

AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

For general information regarding STN implementation of IPC 8

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FILE 'HOME' ENTERED AT 18:08:15 ON 07 MAR 2008

=> file eq

'EG' IS NOT A VALID FILE NAME

SESSION CONTINUES IN FILE 'HOME'

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

0.21

0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 18:08:25 ON 07 MAR 2008
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http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10576194.str

2224

G1:C,N

15

Match level:

normalized bonds :

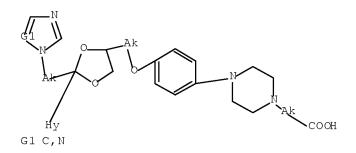
isolated ring systems : containing 1 : 6 : 12 : 18 :

12-13 12-17 13-14 14-15 15-16 16-17

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 28:Atom 29:CLASS

L1 STRUCTURE UPLOADED

=> d 11L1 HAS NO ANSWERS L1STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11 full

FULL SEARCH INITIATED 18:08:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 159 TO ITERATE

100.0% PROCESSED 159 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

L2 0 SEA SSS FUL L1

=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 180.66 180.87

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http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10576194claim1.str

```
chain nodes :
23 24 26 27 37 40 41 43
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 29
30 31 32 33 34
ring/chain nodes :
35 36 38
chain bonds :
1-23 8-17 11-31 14-24 19-23 19-26 21-27 24-27 34-35 35-36 35-43 36-37
36-38 38-40 38-41
ring bonds :
1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 4-5 \quad 6-7 \quad 6-11 \quad 7-8 \quad 8-9 \quad 9-10 \quad 10-11 \quad 12-13 \quad 12-17 \quad 13-14 \quad 14-18 
15
15-16 \quad 16-17 \quad 18-19 \quad 18-22 \quad 19-20 \quad 20-21 \quad 21-22 \quad 29-30 \quad 29-34 \quad 30-31 \quad 31-32 \quad 32-33
33 - 34
exact/norm bonds :
1-2 \quad 1-5 \quad 1-23 \quad 2-3 \quad 3-4 \quad 4-5 \quad 6-7 \quad 6-11 \quad 7-8 \quad 8-9 \quad 8-17 \quad 9-10 \quad 10-11 \quad 11-31 \quad 14-24
18-19 18-22 19-20 19-23 19-26 20-21 21-22 21-27 24-27 34-35 35-36 35-43
36-37 36-38
38-40 38-41
normalized bonds :
12-13 12-17 13-14 14-15 15-16 16-17 29-30 29-34 30-31 31-32 32-33 33-34
isolated ring systems :
containing 1 : 6 : 12 : 18 : 29 :
```

G1:C,N

G2:C,H

```
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom
22:Atom 23:CLASS 24:CLASS 26:Atom 27:CLASS 29:Atom 30:CLASS 31:Atom 32:Atom
33:Atom 34:Atom
```

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 13 full

FULL SEARCH INITIATED 18:12:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 57 TO ITERATE

100.0% PROCESSED 57 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

L4 0 SEA SSS FUL L3

=>

Uploading C:\Program Files\Stnexp\Queries\10576194noB.str

```
chain nodes :
23 24 26 27
ring nodes :
chain bonds :
1-23 8-17 14-24 19-23 19-26 21-27 24-27
ring bonds :
1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 4-5 \quad 6-7 \quad 6-11 \quad 7-8 \quad 8-9 \quad 9-10 \quad 10-11 \quad 12-13 \quad 12-17 \quad 13-14 \quad 14-18 
15
15-16 16-17 18-19 18-22 19-20 20-21 21-22
exact/norm bonds :
1-2 \quad 1-5 \quad 1-23 \quad 2-3 \quad 3-4 \quad 4-5 \quad 6-7 \quad 6-11 \quad 7-8 \quad 8-9 \quad 8-17 \quad 9-10 \quad 10-11 \quad 14-24 \quad 18-19
18-22 19-20 19-23 19-26 20-21 21-22 21-27 24-27
normalized bonds :
12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 : 6 : 12 : 18 :
```

G1:C,N

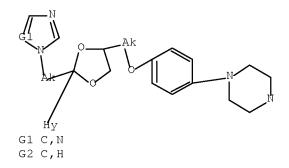
G2:C,H

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 23:CLASS 24:CLASS 26:Atom 27:CLASS

L5 STRUCTURE UPLOADED

=> d 15 L5 HAS NO ANSWERS L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15 full

FULL SEARCH INITIATED 18:16:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2304 TO ITERATE

100.0% PROCESSED 2304 ITERATIONS 12 ANSWERS

SEARCH TIME: 00.00.01

L6 12 SEA SSS FUL L5

=> file caplus

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
SINCE FILE TOTAL
25 SESSION
359.02
539.89

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=> s 16 full

L7 2 L6

=> d ibib abs hitstr tot

L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:598868 CAPLUS Full-text

DOCUMENT NUMBER: 145:180204

TITLE: Novel ketoconazole analogues based on the replacement

of 2,4-dichlorophenyl group with 1,4-benzothiazine

moiety: Design, synthesis, and microbiological

evaluation

AUTHOR(S): Schiaffella, Fausto; Macchiarulo, Antonio; Milanese,

Lara; Vecchiarelli, Anna; Fringuelli, Renata

CORPORATE SOURCE: Department of Drug Chemistry and Technology,

University of Perugia, Perugia, 06100, Italy

SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(15),

5196-5203

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:180204

As a part of a program to develop novel antifungal agents, new compds. which incorporate the 1,4-benzothiazine moiety into the structure of ketoconazole (KTZ) were prepared These compds. were computationally investigated to assess whether the 1,4-benzothiazine moiety was a suitable bioisosteric replacement for the 2,4-dichlorophenyl group of KTZ in order to obtain a more potent inhibition of CYP51 enzyme of Candida albicans. Results of preliminary microbiol. studies show that the racemic cis-7 analog has a good in vivo activity, comparable to that of KTZ, but the best activity was observed in the racemic trans-7 analog.

IT 902799-20-6P 902799-21-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(benzothiazine ketoconazole analogs as antifungal agents)

RN 902799-20-6 CAPLUS

CN Piperazine, 1-acetyl-4-[4-[[(2R,4S)-2-(3,4-dihydro-4-methyl-3-oxo-2H-1,4-benzothiazin-7-yl)-2-(1H-imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 902799-21-7 CAPLUS

CN Piperazine, 1-acetyl-4-[4-[(2R,4R)-2-(3,4-dihydro-4-methyl-3-oxo-2H-1,4-benzothiazin-7-yl)-2-(1H-imidazol-1-ylmethyl)-1,3-dioxolan-4-

yl]methoxy]phenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:395302 CAPLUS Full-text

DOCUMENT NUMBER: 142:447236

TITLE: Preparation of 2-(azolylmethyl)-4-

(piperazinylphenoxymethyl)-1,3-dioxolanes as

antifungals with reduced interaction with metabolic

cytochromes.

INVENTOR(S): Pinori, Massimo; Lattanzio, Maria; Modena, Daniela;

Mascagni, Paolo

PATENT ASSIGNEE(S): Italfarmaco S.p.A., Italy SOURCE: PCT Int. Appl., 27 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.					KIND		DATE		APPLICATION NO.						DATE		
WO 2005040156					A1		20050506		WO 2004-EP11667						20041014		
	W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NΙ,
		NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	ΙT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,
		SN,	TD,	ΤG													
CA 2542361					A1		2005	0506	CA 2004-2542361						20041014		
EP	P 1673368				A1		20060628			EP 2004-790506					20041014		
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	FI,	RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK				
CN 1867565					Α		2006	1122	CN 2004-80030607					20041014			
BR 2004015319					Α	20061205			BR 2004-15319					20041014			
JP 2007533638					T	20071122			JP 2006-534715					20041014			

IN 2006DN01807 A 20070810 IN 2006-DN1807 20060403 US 2007129376 A1 20070607 US 2006-576194 20060417 PRIORITY APPLN. INFO.: IT 2003-MI2020 A 20031017 WO 2004-EP11667 W 20041014

Ι

OTHER SOURCE(S): CASREACT 142:447236; MARPAT 142:447236 GI

AB Title compds. [I; A = N, CH; Het = heteroaryl optionally substituted by ≥1 5-6 membered aromatic rings; B = alkanoate, 4-C6H4NR2CONR1R3; R1 = H, (substituted) alkyl; R2, R3 = H, alkyl; R2R3 = CH:N, CH:CH, CH2CH2], were prepared Thus, 2, 4-dihydro-4-[4-[4-(4-hydroxyphenyl)-1- piperazinyl]phenyl]-2-(1-methylpropyl)-3H-1,2,4-triazol-3-one in DMF was treated with KOCMe3 and then with cis-[2-(pyridin-2-yl)-2-(1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-ylmethyl] tosylate in DMF followed by heating at 130° for 3 h to give 28% cis-<math>4-[4-[4-[4-[2-(pyridin-2-yl)-2-(1H- 1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-ylmethoxy]phenyl]-1- piperazinyl]phenyl]-2-(1-methoxypropyl)-2,4-dihydro-3H-1,2,4-triazol-3- one. The latter at 50 mg/kg/day in mice infected with Candida albicans gave a mean survival time of 9.1 days, vs. 5.3 for untreated controls.

IT 851341-62-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of azolylmethylpiperazinylphenoxymethyldioxolan

es as antifungals with reduced interaction with metabolic cytochromes)

RN 851341-62-3 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-2-(1-methylpropyl)-4-[4-[4-[4-[4-[(2R,4R)-2-(2-pyridinyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]phenyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

IT 851341-72-5P 851341-73-6P 851341-74-7P 851341-75-8P 851341-76-9P 851341-77-0P 851341-78-1P 851341-79-2P 851341-80-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of azolylmethylpiperazinylphenoxymethyldioxolanes as antifungals with reduced interaction with metabolic cytochromes)

RN 851341-72-5 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-2-(1-methylpropyl)-4-[4-[4-[4-[4-[4-[(2R,4S)-2-(4-pyridinyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]phenyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 851341-73-6 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-2-(1-methylpropyl)-4-[4-[4-[4-[4-[4-[(2R,4S)-2-(3-pyridinyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]phenyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 851341-74-7 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-2-(1-methylpropyl)-4-[4-[4-[4-[4-[(2R,4R)-2-(2-thiazolyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]phenyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 851341-75-8 CAPLUS

Absolute stereochemistry.

RN 851341-76-9 CAPLUS

Absolute stereochemistry.

RN 851341-77-0 CAPLUS

Absolute stereochemistry.

RN 851341-78-1 CAPLUS

Absolute stereochemistry.

RN 851341-79-2 CAPLUS

Relative stereochemistry.

RN 851341-80-5 CAPLUS

Relative stereochemistry.

PAGE 1-A

PAGE 1-B

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 18:08:15 ON 07 MAR 2008)

FILE 'REGISTRY' ENTERED AT 18:08:25 ON 07 MAR 2008

L1 STRUCTURE UPLOADED

L2 0 S L1 FULL

FILE 'REGISTRY' ENTERED AT 18:12:15 ON 07 MAR 2008

L3 STRUCTURE UPLOADED

L4 0 S L3 FULL

L5 STRUCTURE UPLOADED

L6 12 S L5 FULL

FILE 'CAPLUS' ENTERED AT 18:16:13 ON 07 MAR 2008

L7 2 S L6 FULL

=> log y

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 556.55 16.66 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -1.60-1.60

STN INTERNATIONAL LOGOFF AT 18:23:30 ON 07 MAR 2008